# Stable and Efficient Galerkin Reduced Order Models for Non-Linear Fluid Flow

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## 1 Introduction

Despite the development of increasingly sophisticated "high-fidelity" computational fluid dynamics (CFD) tools and improved numerical methods, direct simulation of three-dimensional unsteady flow at high Reynolds number is in practice often too computationally expensive for use in a design or analysis setting. This situation has motivated the formulation of techniques that retain the essential physics and dynamics of a high-fidelity model, but at a much lower computational cost. The basic idea of these "Reduced Order Models" (ROMs) is to use a relatively small number of solutions generated by a high-fidelity simulation to construct a model that is much cheaper computationally, one that could be solved in real or near-real time for use in applications where simulations must be run for on-the-spot decision making, optimization, and/or control. Such ROMs can enable and enhance the understanding of complex fluid systems and non-linear dynamics in turbulent flows at a relatively low computational cost.

In the present work, a Proper Orthogonal Decomposition (POD)/Galerkin reduced order model (ROM) for the full non-linear compressible Navier-Stokes equations is formulated. A reduced model for these formidable equations is desired to have the following properties:

1. The ROM numerical solution should be bounded in a way that is consistent with the behavior of the exact solutions to the governing equations, i.e., it should be stable.
2. The ROM should be computationally efficient.

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It was shown in earlier works [1, 2, 3, 11] that maintaining a proper energy balance is crucial to building a stable reduced order model. It was also shown that the inner product used to define the Galerkin projection is closely tied to the stability of the resulting model. For the non-linear Euler or Navier-Stokes equations, the energy method goes hand in hand with the second law of thermodynamics, or the Clausius-Duhem inequality, which essentially states that the entropy of a system is non-decreasing. Our aim here is to develop a transformation (symmetrization) and define an inner product such that the Clausius-Duhem inequality is necessarily satisfied for a Galerkin ROM constructed for the compressible Navier-Stokes equations. This transformation leads to the introduction of additional non-linearities into the governing system of equations in the so-called "entropy variables". To maintain efficiency, a formulation in which the non-linear terms are handled using the "best points interpolation method" (BPIM) proposed by Peraire, Nguyen *et. al.* in [14, 15] is developed. To gauge the viability of the POD basis for non-linear fluid equations supporting weak shocks and rarefactions, and to study numerically the effectiveness of the BPIM when applied to problems whose solutions exhibit these characteristics, some POD/Galerkin ROMs are constructed for the viscous Burgers' equation and other conservation laws.

## 2 The POD/Galerkin Approach for Model Reduction

This section contains a brief overview of the Proper Orthogonal Decomposition (POD)/Galerkin method for reducing the order of a complex physical system governed by a general set of PDEs. The approach consists of two steps:

1. Calculation of a reduced basis using the proper orthogonal decomposition of an ensemble of flowfield realizations, followed by
2. The Galerkin projection of the governing partial differential equations (PDEs) onto the reduced basis.

When successful, the result of this procedure is a set of time-dependent ordinary differential equations (ODEs) in the modal amplitudes that accurately describes the flow dynamics of the full system of PDEs for some limited set of flow conditions.

The first step in the model reduction procedure is the calculation of a reduced basis using the POD of an ensemble of realizations from a high-fidelity simulation. Discussed in detail in Lumley [13] and Holmes *et. al.* [9], POD is a mathematical procedure that, given an ensemble of data, constructs a basis for that ensemble that is optimal in the sense that it describes more energy (on average) of the ensemble than any other linear basis of the same dimension $M$. In the present context, the ensemble $\{u^k(x) : k = 1,\ldots,N\}$ is a set of $N$ instantaneous snapshots of a high fidelity numerical solution field. Mathematically, POD seeks an $M$-dimensional ($M << N$) subspace $\mathscr{H}^M(\Omega)$ spanned by the set $\{\phi_i\}$ such that the projection of the difference between the ensemble $u^k$ and its projection onto $\mathscr{H}^M(\Omega)$ is minimized on average. It is a well-known result [1, 9, 12, 17] that the solution to this optimization problem reduces to the eigenvalue problem $\mathscr{R}\phi = \lambda\phi$ where $\mathscr{R} \equiv \langle u^k \otimes u^k \rangle$ is a self-adjoint and positive semi-definite operator. If it is assumed that $\mathscr{R}$ is compact, then there exists a countable set of non-negative eigenvalues $\lambda_i$ with associated eigenfunctions $\phi_i$. It can be shown [9, 13] that the set of $M$ eigenfunctions, or POD modes, $\{\phi_i : i = 1,2,\ldots,M\}$ corresponding to the $M$ largest eigenvalues of $\mathscr{R}$ is precisely the set of $\{\phi_i\}$ that solves the POD eigenvalue problem. Given this basis, the numerical ROM solution $u_M$ can be represented as a linear combination of POD modes

$$u_M(x,t) = \sum_{j=1}^{M} a_j(t)\phi_j(x), \tag{1}$$

where the $a_j(t)$ are the so-called ROM coefficients, to be solved for in the ROM.

The second step in constructing a ROM involves projecting the governing system of PDEs onto the POD basis $\{\phi_i\}$ in some appropriate inner product, denoted generically (for now) by $(\cdot,\cdot)$. In this step, the full-system dynamics are effectively translated to the implied dynamics of the POD modes. If the governing system of equations for the state variable vector $u$ has the form

$$\frac{\partial u}{\partial t} = \mathscr{L}u + \mathscr{N}_2(u,u) + \mathscr{N}_3(u,u,u), \tag{2}$$

where $\mathscr{L}$ is a linear differential operator, and $\mathscr{N}_2$ and $\mathscr{N}_3$ are (non-linear) quadratic and cubic operators respectively, then the Galerkin projection of (2) onto the POD mode $\phi_j$ for $j = 1,2,...,M$ is

$$\left(\phi_j, \frac{\partial u_M}{\partial t}\right) = (\phi_j, \mathscr{L}u_M) + (\phi_j, \mathscr{N}_2(u_M,u_M)) + (\phi_j, \mathscr{N}_3(u_M,u_M,u_M)). \tag{3}$$

Substituting the POD decomposition of $u$ (1) into (3) and applying the orthonormality property of the basis functions $\phi_i$ in the inner product $(\cdot,\cdot)$ gives a set of time-dependent ordinary differential equations (ODEs) in the modal amplitudes (also referred to as the ROM coefficients) that accurately describes the flow dynamics of the full system of PDEs for some limited set of flow conditions:

$$\begin{aligned}\frac{da}{dt} \equiv \dot{a}_j \quad &= \sum_{l=1}^{M} a_l(\phi_j, \mathscr{L}(\phi_l)) + \sum_{l=1}^{M}\sum_{m=1}^{M} a_l a_m (\phi_j, \mathscr{N}_2(\phi_l,\phi_m)) \\ &\quad + \sum_{l=1}^{M}\sum_{m=1}^{M}\sum_{n=1}^{M} a_l a_m a_n (\phi_j, \mathscr{N}_3(\phi_l,\phi_m,\phi_n)),\end{aligned} \tag{4}$$

for $j = 1,2,\ldots,M$.

It is emphasized that the approach described herein is based on a Galerkin projection of the governing partial differential equations, in common with the perspective of, for example, [1, 2, 11, 12]. This "continuous projection" approach differs from many POD/Galerkin applications, where the semi-discrete representation of the governing equations is projected, and numerical analysis proceeds from the perspective of a dynamical system of ordinary differential equations. The continuous projection approach has the advantage that the ROM solution behavior can be examined using methods that have traditionally been used for numerical analysis of spectral approximations to partial differential equations [7, 6], such as the techniques employed herein in examining stability. Unlike the discrete approach, however, in the continuous approach, boundary condition terms present in the discretized equation set are *not* in general inherited by the ROM.

## 3 Interpolation of Non-Linear Terms

The efficiency in solving the reduced ODE system (4) depends on the nature of the non-linearities in the original set of equations (2). Consider the general non-linear initial boundary value problem (IBVP):

$$\frac{\partial u}{\partial t} + \mathscr{L}u + \mathscr{N}(u) = f, \tag{5}$$

where $\mathscr{L}$ is a linear operator, $\mathscr{N}$ is a non-linear operator, and $f$ is some source depending on space only (not a function of $u$). Projecting (5) onto the $j^{th}$ POD mode, for $j = 1,...,M$ modes gives rise to a system of ODEs of the form

$$\dot{\mathbf{a}}_M = \mathbf{F} - \mathbf{L}\mathbf{a}_M - \mathbf{N}(\mathbf{a}_M), \tag{6}$$

where $\mathbf{a}_M^T \equiv \begin{pmatrix} a_1, & \ldots & a_M \end{pmatrix}$, $L_{ij} \equiv (\mathscr{L}\phi_j, \phi_i)$, $F_i \equiv (f, \phi_i)$ for $i, j = 1,...,M$ and

$$N_i(\mathbf{a}_M) \equiv \left(\mathscr{N}\left(\sum_{k=1}^{M} a_k\phi_k\right), \phi_i\right), \qquad i = 1,...,M. \tag{7}$$

The inner products in (7) *cannot* be pre-computed prior to time-integration of the ROM system (6) if $\mathscr{N}$ contains a strong, e.g., a non-polynomial, non-linearitity, as could (and would) be done in the case of linear equations. When $\mathscr{N}$ contains a polynomial non-linearity, the required inner products *could* be pre-computed, as illustrated in (4) for a problem with a quadratic and a cubic non-linearity. The cost of performing the required inner product, however, for an operator $\mathscr{N}$ that contains a polynomial non-linearity of order $p > 1$ is in general $\mathscr{O}(N^{p+1})$, where $N$ is the number of spatial discretization points. Thus, "direct" treatment, or computation, of these inner products can greatly reduce the efficiency of this ROM, and motivates the consideration of some alternative way to handle the non-linearity in (5).

To recover efficiency, the "best points" interpolation of [14, 15], a technique based on a coefficient function approximation for the non-linear terms in (5), is employed. The general procedure is outlined in this section.

Suppose $K$ snapshots have been taken of the primal unknown field, at $K$ different times:

$$\mathscr{S}^u \equiv \{\xi_k^u(x) = u_h^k(x) : 1 \leq k \leq K\}. \tag{8}$$

Here, the $u_h^k(s)$ are vectors of state variables at grid point locations, each containing a single solution (snapshot) from the numerical simulation (Step 1 of the POD/Galerkin approach for model reduction outlined in Section 2).

Given this set of snapshots of the primal unknown field $u$, the following set of snapshots of the non-linear function $\mathscr{N}$ appearing in (5) are constructed:

$$\mathscr{S}^{\mathscr{N}} \equiv \{\xi_k^{\mathscr{N}}(x) = \mathscr{N}(u_h^k(x)) : 1 \leq k \leq K\}. \tag{9}$$

The best approximations of the elements in the snapshot set are now defined as:

$$\mathscr{N}_M^*(u_h^k(\cdot)) = \arg \min_{w_M \in \text{span}\{\phi_1^{\mathscr{N}},\ldots,\phi_M^{\mathscr{N}}\}} ||\mathscr{N}(u_h^k(\cdot)) - w_M||, \quad 1 \leq k \leq K, \tag{10}$$

where $\{\phi_m^{\mathscr{N}}\}_{m=1}^M$ is an orthonormal basis for $\mathscr{N}$, and $||\cdot||$ denotes the norm induced by the inner product $(\cdot,\cdot)$ in which the POD basis is constructed. Orthonormality of the $\phi_m^{\mathscr{N}}$ implies that

$$\mathscr{N}_M^*(u_h^k(x)) = \sum_{m=1}^M \alpha_m^k \phi_m^{\mathscr{N}}(x), \quad 1 \leq k \leq K, \tag{11}$$

where

$$\alpha_m^k = (\phi_m^{\mathscr{N}}, \mathscr{N}(u_h^k(\cdot))), \quad m = 1,\ldots,M, 1 \leq k \leq K. \tag{12}$$

The "best" interpolation points [14, 15] $\{x_m^{bp}\}_{m=1}^M$ are defined as the solution to the following optimization problem:

$$\begin{array}{c} \min_{x_1^{bp},\ldots,x_M^{bp} \in \Omega} \sum_{k=1}^K \left|\left| \mathscr{N}_M^*(u_h^k(\cdot)) - \sum_{m=1}^M \beta_m^k(x_1^{bp},\ldots,x_M^{bp}) \phi_m^{\mathscr{N}} \right|\right|^2, \\ \sum_{n=1}^M \phi_n^{\mathscr{N}}(x_m^{bp}) \beta_n^k(x_1^{bp},\ldots,x_M^{bp}) = \mathscr{N}(u_h^k(x_m^{bp})), \quad 1 \leq m \leq M, 1 \leq k \leq K. \end{array} \tag{13}$$

Substituting (11) into (13) and invoking the orthonormality of the $\{\phi_m^{\mathscr{N}}\}_{m=1}^M$:

$$\begin{array}{c} \min_{x_1^{bp},\ldots,x_M^{bp} \in \Omega} \sum_{k=1}^K \sum_{m=1}^M (\alpha_m^k - \beta_m^k(x_1^{bp},\ldots,x_M^{bp}))^2, \\ \sum_{n=1}^M \phi_n^{\mathscr{N}}(x_m^{bp}) \beta_n^k(x_1^{bp},\ldots,x_M^{bp}) = \mathscr{N}(u_h^k(x_m^{bp})), \quad 1 \leq m \leq M, 1 \leq k \leq K, \end{array} \tag{14}$$

i.e., the set of points $\{x_m^{bp}\}_{m=1}^M$ is determined to minimize the average error between the interpolants $\mathscr{N}_M(\cdot)$ and the best approximations $\mathscr{N}_M^*(\cdot)$. The solution to the least-square optimization problem (14) can be found

using the Levenberg-Marquardt (LM) algorithm. The optimal solution to (14) is typically reached in less than fifteen iterations of the LM algorithm [15].

Given the "best points" for $\mathscr{N}$, i.e., the solutions to (14) (or any set of interpolation points), denoted by $\{x_m^{\mathscr{N}}\}_{m=1}^M$, it is straight forward to apply the interpolation procedure outlined in [14, 15] to the non-linear function $\mathscr{N}(u)$ that appears in (5). The first step is to compute snapshots for the non-linear function $\mathscr{N}$ in (5). From these snapshots the interpolation points $\{x_m^{\mathscr{N}}\}_{m=1}^M$ are determined following the approach outlined above and in Section 2 of [15]. Given $\{x_m^{\mathscr{N}}\}_{m=1}^M$ and $\{\phi_m^{\mathscr{N}}\}_{m=1}^M$, the so-called "cardinal functions" $\{\psi_m^{\mathscr{N}}\}_{m=1}^M$ are computed by solving the following linear system[1]

$$\boldsymbol{\phi}_M^{\mathscr{N}}(x) = \mathbf{A}\boldsymbol{\psi}_M^{\mathscr{N}}(x), \tag{15}$$

where $\boldsymbol{\phi}_M^{\mathscr{N}}(x) = (\phi_1^{\mathscr{N}}(x), ..., \phi_M^{\mathscr{N}}(x))^T$ and $\boldsymbol{\psi}_M^{\mathscr{N}}(x) = (\psi_1^{\mathscr{N}}(x), ..., \psi_M^{\mathscr{N}}(x))^T$, and $A_{ij} = \phi_j^{\mathscr{N}}(x_i)$, with the cardinal functions satisfying $\psi_j(z_i) = \delta_{ij}$.

Given the interpolation points $\{x_m^{\mathscr{N}}\}$ and the cardinal functions $\{\psi_m^{\mathscr{N}}\}$, the non-linear function $\mathscr{N}$ can be approximated as:

$$\mathscr{N}(u) \approx \mathscr{N}_M(u) = \sum_{m=1}^{M} \mathscr{N}(u(x_m^{\mathscr{N}}))\psi_m^{\mathscr{N}} \in \mathbb{R}, \tag{16}$$

so that

$$\mathscr{N}_M = \sum_{m=1}^{M} \mathscr{N}\left(\sum_{n=1}^{M} a_n(t)\phi_n(x_m^{\mathscr{N}})\right)\psi_m^{\mathscr{N}}, \tag{17}$$

where $\{\phi_m(x) : m = 1, ..., M\}$ is an orthonormal basis for the primal unknown $u$, computed from the snapshots (8).

The projection of $\mathscr{N}_M$ onto the $l^{th}$ POD mode for $u$ can be written in matrix/vector form. To do this, note that, for a general function $\mathscr{N}_M$ and for $l = 1, ..., M$:

$$\begin{aligned}(\phi_l, \mathscr{N}_M) &= \left(\phi_l, \textstyle\sum_{m=1}^M \mathscr{N}\left(\sum_{n=1}^M a_n\phi_n(x_m^{\mathscr{N}})\right)\psi_m^{\mathscr{N}}\right) \\ &= \textstyle\sum_{m=1}^M \left[\int_\Omega \phi_l\psi_m^{\mathscr{N}} d\Omega\right] \mathscr{N}\left(\sum_{n=1}^M a_n\phi_n(x_m^{\mathscr{N}})\right).\end{aligned} \tag{18}$$

(18) is a matrix/vector product of the form $\mathbf{G}\mathscr{N}\left(\sum_{n=1}^M a_n\phi_n(x_m^{\mathscr{N}})\right)$ where

$$G_{nm} = \int_\Omega \phi_n\psi_m^{\mathscr{N}} d\Omega, \tag{19}$$

for $1 \le m, n \le M$ (so that $\mathbf{G} \in \mathbb{R}^{M\times M}$).

It follows that, with the interpolation procedure employed here, our ODE system for the ROM coefficients is not (6) but rather

$$\dot{\mathbf{a}}_M = \mathbf{F} - \mathbf{L}\mathbf{a}_M - \mathbf{G}\mathscr{N}(\mathbf{D}^{\mathscr{N}}\mathbf{a}_M), \tag{20}$$

where the entries of $\mathbf{G}$ are given by (19), and $D_{ij}^{\mathscr{N}} = \phi_j(x_i^{\mathscr{N}})$ for $i, j = 1, ..., M$.

Essentially, in the BPIM, recomputation of inner products (projection) of the non-linear terms at each time (or Newton) step is replaced by evaluation of the basis functions at the (pre-computed) interpolation points. There is also a matrix inversion (15) involved in solving for the cardinal functions $\{\psi_m^{\mathscr{N}}\}_{m=1}^M$ (15), an $\mathscr{O}(N^3)$ operation. The computational complexity of the "best points" interpolation algorithm is discussed in detail

[1]Note that, for $\mathbf{A}$ to be invertible, the number of interpolation points must be equal to the number of modes $M$. A non-linear least squares optimization problem may be formulated if it is desired to have more interpolation points than modes $M$, but this latter approach is not considered in the present work.

in [14, 15]. For $M \leq N$, the complexity of the online stage of the interpolation algorithm is of $\mathcal{O}(N^3)$. It follows that, given a set of interpolation points, the interpolation procedure outlined above improves computational efficiently over the "direct" treatment of the non-linear term (6) if the non-linearity $\mathcal{N}(u)$ is non-polynomial, or a polynomial of degree three or higher.

# 4 Inner Product and Entropy-Stability

The discussion in Sections 2 and 3 has assumed a generic inner product $(\cdot,\cdot)$. As it turns out, the inner product employed in the Galerkin projecion step is closely related to the numerical stability of the resulting reduced order model. This is because the inner product is a mathematical expression for the energy in the ROM. The majority of POD/Galerkin models for fluid flow use as the governing equation set the incompressible Navier Stokes equations. Because in these models the solution vector is taken to be the velocity vector $\mathbf{u}$, so that $||\mathbf{u}||_{L^2(\Omega)}$ is a measure of the global kinetic energy in the domain $\Omega$, the natural choice of inner product for these equations is the $L^2(\Omega)$ inner product. In effect, the $L^2(\Omega)$ inner product is physically sensible for these equations: the POD modes optimally represent the kinetic energy present in the ensemble from which they are generated. The same is *not* true for other equations arising in fluid mechanics. For example, as shown in [1, 2, 3, 11], the $L^2(\Omega)$ inner product does not correspond to an energy integral for the linearized compressible Euler equations, meaning if it is selected as the inner product defining the projection, the ROM does not satisfy the energy conservation relation implied by the governing equations. For these equations, a symmetry transformation is required to yield a stable approximation. This transformation motivates the construction of a weighted $L^2(\Omega)$ inner product that guarantees certain stability bounds satisfied by the ROM solution [1, 2, 3, 11].

The aim of the present work is to employ a stability analysis similar to that in [1, 2, 3, 11] to develop a non-linear Galerkin ROM whose numerical solution is bounded in a way consistent with behavior of exact solutions of the original differential equations, i.e. it is stable. As discussed in [5, 10], stability can be ensured by the energy method. For the full (non-linear) Euler or Navier-Stokes equations, the energy method is closely tied to the second law of thermodynamics, or the Clausius-Duhem inequality, namely

$$\frac{d}{dt}\int_{\Omega}\rho\eta\, d\Omega \geq -\int_{\partial\Omega_W}\frac{q_i n_i}{\theta}dS, \tag{21}$$

where $\eta$ is the thermodynamic entropy density per unit mass (Table 1). (21) essentially states that the entropy of the system is non-decreasing. For the non-linear equations of fluid mechanics, energy estimates, or the satisfaction of the entropy inequality (21), imply that the semi-discrete solutions possess stability properties akin to those of the exact solutions of the governing equations [5, 10]. Solutions that satisfy (21) will be referred to as "entropy-stable". The aim of Section 5 is to develop a transformation (symmetrization) and define an inner product such that the Clausius-Duhem inequality (21) is necessarily satisfied for a Galerkin ROM constructed for the compressible Navier-Stokes equations.

# 5 An Entropy-Stable and Efficient Reduced Order Model (ROM) for the 3D Compressible Navier-Stokes Equations

## 5.1 Governing Equations

In terms of the so-called conservation variables $\mathbf{U}$, the Navier-Stokes equations for compressible flow can be written as (neglecting forces) [10]:

$$\mathbf{U}_{,t} + \mathbf{F}_{i,i} = \mathbf{F}^v_{i,i} + \mathbf{F}^h_{i,i}, \tag{22}$$

where, in three-dimensions (3D):

$$\mathbf{U} \equiv \begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{pmatrix} \equiv \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho e \end{pmatrix}, \tag{23}$$

$$\mathbf{F}_i = u_i \mathbf{U} + p \begin{pmatrix} 0 \\ \delta_{1i} \\ \delta_{2i} \\ \delta_{3i} \\ u_i \end{pmatrix}, \quad \mathbf{F}^v_i = \begin{pmatrix} 0 \\ \tau_{1i} \\ \tau_{2i} \\ \tau_{3i} \\ \tau_{ij} u_j \end{pmatrix}, \quad \mathbf{F}^h_i = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -q_i \end{pmatrix}, \tag{24}$$

for $i = 1,2,3$. $\mathbf{F}_i$ is known as the convective or Euler flux, $\mathbf{F}^v_i$ is the viscous flux, and $\mathbf{F}^h_i$ is the heat flux. The variables and parameters appearing in (23)–(24) are defined in Table 1 of the Appendix. The specific heats are assumed to be positive constants. Moreover, we require that $\mu \geq 0$, $\lambda + \frac{2}{3}\mu \geq 0$, and $\kappa \geq 0$.

(22) is the conservative form of the 3D compressible Navier-Stokes equations. These equations can also be written in non-conservative form as

$$\mathbf{U}_{,t} + \mathbf{A}_i \mathbf{U}_{,i} = (\mathbf{K}_{ij} \mathbf{U}_{,j})_{,i}, \tag{25}$$

where $\mathbf{A}_i \equiv \mathbf{A}_i(\mathbf{U})$, $\mathbf{K}^v_{ij} \equiv \mathbf{K}^v_{ij}(\mathbf{U})$ and $\mathbf{K}^h_{ij} \equiv \mathbf{K}^h_{ij}(\mathbf{U})$ are defined by

$$\mathbf{F}_{i,i} = \mathbf{F}_{i,\mathbf{U}} \mathbf{U}_{,i} \equiv \mathbf{A}_i \mathbf{U}_{,i}, \quad \mathbf{F}^v_i \equiv \mathbf{K}^v_{ij} \mathbf{U}_{,j}, \tag{26}$$

$$\mathbf{F}^h_i \equiv \mathbf{K}^h_{ij} \mathbf{U}_{,j}, \quad \mathbf{K}_{ij} \equiv \mathbf{K}^v_{ij} + \mathbf{K}^h_{ij}. \tag{27}$$

Neglecting for now the far-field boundary conditions, so that only the solid wall boundary conditions are considered explicitly, and denoting the solid wall boundary of the domain $\Omega$ by $\partial\Omega_W \equiv \partial\Omega$, the relevant boundary conditions at the solid wall are:

$$\begin{array}{lll} \text{no slip BC:} & \mathbf{u} = \mathbf{0}, & \text{on } \partial\Omega_W, \\ \text{adiabatic wall BC:} & \nabla\theta \cdot \mathbf{n} = 0, & \text{on } \partial\Omega_W. \end{array} \tag{28}$$

Since the POD basis functions may not satisfy the no-slip condition at the wall, it is often desirable to implement a no-penetration boundary condition at the wall as well:

$$\text{no-penetration BC:} \quad \mathbf{u} \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega_W. \tag{29}$$

## 5.2 Entropy Variables for the 3D Compressible Navier-Stokes Equations

To develop a Clausius-Duhem inequality-preserving Galerkin projection of the equations (25), one begins by introducing a change of variables $\mathbf{U} \rightarrow \mathbf{V}$:

$$\mathbf{U} = \mathbf{U}(\mathbf{V}), \tag{30}$$

where $\mathbf{V}$ are the so-called "entropy variables". In terms of the entropy variables $\mathbf{V}$, the equations of interest (25) are:

$$\mathbf{A}_0\mathbf{V}_{,t} + \tilde{\mathbf{A}}_i\mathbf{V}_{,i} - (\tilde{\mathbf{K}}_{ij}\mathbf{V}_{,j})_{,i} = \mathbf{0}, \tag{31}$$

where[2]

$$\mathbf{A}_0 \equiv \mathbf{U}_{,\mathbf{V}}, \quad \tilde{\mathbf{A}}_i \equiv \mathbf{A}_i\mathbf{A}_0, \quad \tilde{\mathbf{K}}_{ij} \equiv \mathbf{K}_{ij}\mathbf{A}_0. \tag{32}$$

It is well-known that the matrices $\mathbf{A}_i$ in (25) are non-symmetric. However, it is also well-known that all linear combinations of the $\mathbf{A}_i$ possess real eigenvalues and a complete set of eigenvectors, meaning $\mathbf{U}_{,t} + \mathbf{A}_i\mathbf{U}_{,i} = \mathbf{0}$ constitutes a hyperbolic system of conservation laws. The change of variables (30) is sought such that:

1. The matrices $\mathbf{A}_0$ and $\tilde{\mathbf{A}}_i$ are symmetric, and
2. The matrix

$$\tilde{\mathbf{K}} \equiv \begin{pmatrix} \tilde{\mathbf{K}}_{11} & \tilde{\mathbf{K}}_{12} & \tilde{\mathbf{K}}_{13} \\ \tilde{\mathbf{K}}_{21} & \tilde{\mathbf{K}}_{22} & \tilde{\mathbf{K}}_{23} \\ \tilde{\mathbf{K}}_{31} & \tilde{\mathbf{K}}_{32} & \tilde{\mathbf{K}}_{33} \end{pmatrix}, \tag{33}$$

   is symmetric positive semi-definite.

If the transformation (30) is such that these properties hold, the resulting system in the entropy variables will be a symmetric hyperbolic system.

Following the symmetrization approaches of [5, 10], the change of variables (30) is defined with the help of so-called generalized entropy functions. A generalized entropy function $H \equiv H(\mathbf{U})$ is by definition a function that satisfies the following two conditions [10]:

1. $H$ is convex[3].
2. There exist scalar-valued function $\sigma_i \equiv \sigma_i(\mathbf{U})$, $i = 1,2,3$, referred to as entropy fluxes, such that

$$H_{,\mathbf{U}}\mathbf{A}_i = \sigma_{i,\mathbf{U}}. \tag{34}$$

The following theorems, quoted from [8], delineate the relationship between symmetric hyperbolic systems and generalized entropy functions, and will be employed in our symmetrization of the equations (25):

**Theorem 3.2.1 (Mock).** *A hyperbolic system of conservation laws possessing a generalized entropy function becomes symmetric under the change of variables*

$$\mathbf{V}^T = H_{,\mathbf{U}}. \tag{35}$$

**Theorem 3.2.2 (Godunov).** *If a hyperbolic system can be symmetrized by introducing a change of variables, then a generalized entropy function and corresponding entropy fluxes exist for this system.*

[2] Explicit expressions of the symmetrized matrices (32) will be given in the final conference paper manuscript.

[3] The convexity of $H$ is equivalent to the positive-definiteness of $\mathbf{A}_0$, since $\mathbf{A}_0^{-1} = \mathbf{V}_{,\mathbf{U}} = H_{,\mathbf{UU}}$.

For the compressible Navier-Stokes equations (25), appropriate choices for the entropy flux and entropy function are

$$\sigma_i = Hu_i, \quad H = -\rho g(s) \equiv -\rho s, \tag{36}$$

respectively [8, 10]. Here $s$ is the non-dimensional entropy, $s = \eta/c_v$ (Table 1), which satisfies the well-known Gibbs equation $s = \ln(p\rho^{-\gamma}) + \text{const}$.

With the choice of affine entropy flux (36), the transformation $\mathbf{U} \rightarrow \mathbf{V}$ (35) is given by

$$\mathbf{V} = \frac{1}{\rho_1} \begin{pmatrix} -U_5 + \rho_1(\gamma + 1 - s) \\ U_2 \\ U_3 \\ U_4 \\ -U_1 \end{pmatrix}, \tag{37}$$

where

$$s = \ln\left[\frac{(\gamma-1)\rho_1}{U_1^\gamma}\right], \quad \rho_1 = U_5 - \frac{1}{2U_1}(U_2^2 + U_3^2 + U_4^2). \tag{38}$$

The inverse mapping $\mathbf{V} \rightarrow \mathbf{U}$ is given by

$$\mathbf{U} = \rho_1 \begin{pmatrix} -V_5 \\ V_2 \\ V_3 \\ V_4 \\ 1 - \frac{1}{2V_5}(V_2^2 + V_3^2 + V_4^2) \end{pmatrix} \tag{39}$$

where

$$\rho_1 = \left[\frac{\gamma-1}{(-V_5)^\gamma}\right]^{1/(\gamma-1)} \exp\left(\frac{-s}{\gamma-1}\right) \tag{40}$$

$$s = \gamma - V_1 + \frac{1}{2V_5}(V_2^2 + V_3^2 + V_4^2) \tag{41}$$

### 5.3 Entropy Stable Galerkin Projection of the Compressible Navier-Stokes Equations

The stability of the Galerkin projection in the $L_2(\Omega)$ inner product of the symmetrized compressible Navier-Stokes equations (31) with boundary conditions (28) is now examined. Assume the entropy variables have been expanded in a vector basis $\{\boldsymbol{\phi}_i\}_{i=1}^M \in \mathbb{R}^5$:

$$\mathbf{V}(\mathbf{x},t) \approx \mathbf{V}_M(\mathbf{x},t) = \sum_{m=1}^{M} a_m(t)\boldsymbol{\phi}_m(\mathbf{x}), \tag{42}$$

where the $a_m(t)$ are the modal amplitudes (or ROM coefficients) to be solved for, and that the basis $\{\boldsymbol{\phi}_i\}_{i=1}^M$ is orthonormal in the $L_2(\Omega)$ inner product, so that $(\boldsymbol{\phi}_i, \boldsymbol{\phi}_j) = \delta_{ij}$ for all $i, j = 1, ..., M$.

The Galerkin projection is termed "entropy-stable" if it satisfies the Clausius-Duhem entropy inequality (21), or the second law of thermodynamics. Per the discussion in [5, 10], it is shown in Theorem 5.3.1 that the change of variables (37) is such that when the transformed equations (31) are projected onto a POD mode, the Clausius-Duhem inequality is respected *ab initio* for all numerical solutions.

**Theorem 5.3.1.** *Consider the symmetrized compressible 3D Navier-Stokes equations* (31) *in an open bounded domain* $\Omega \subset \mathbb{R}^3$*, with the no-slip and adiabatic wall boundary condition* (28) *on the boundary* $\partial\Omega_W$*. Define the transformation* $\mathbf{U} \to \mathbf{V}$ *given by the entropy flux* (36)*, so that the relationship between* $\mathbf{U}$ *and the entropy variables* $\mathbf{V}$ *is* (37)*. Then the Galerkin projection onto a POD mode* $\boldsymbol{\phi}_j$ *of* (31) *with boundary conditions* (28) *in the* $L^2(\Omega)$ *inner product is "entropy stable" (i.e.., satisfies the entropy estimate* (21)*) if the POD modes* $\boldsymbol{\phi}_j$ *satisfy the no-slip condition on* $\partial\Omega_W$*, i.e., if* $\phi_j^2 = \phi_j^3 = \phi_j^4 = 0$ *for* $j = 1,...,M$ *where* $\phi_j^i$ *denotes the* $i^{th}$ *component of* $\boldsymbol{\phi}_j$ *for* $i = 1,...,5$*, with entropy estimate*

$$\frac{d}{dt}\int_\Omega \rho\eta d\Omega \geq 0. \tag{43}$$

*Proof.* For brevity, the proof of Theorem 5.3.1 is omitted from the abstract. It will be included in the final conference paper. □

## 5.4 Weak Formulation and Discrete ROM System

An efficient implementation of the ROM for the transformed equations (31) with boundary conditions (28) and (29) is now outlined.

Introducing the shorthand, for $\mathbf{V}_1, \mathbf{V}_2 \in \mathbb{R}^5$:

$$(\mathbf{V}_1, \mathbf{V}_2) \equiv \int_\Omega \mathbf{V}_1^T \mathbf{V}_2 d\Omega, \quad \langle \mathbf{V}_1, \mathbf{V}_2 \rangle_{\partial\Omega_W} \equiv \int_{\partial\Omega_W} \mathbf{V}_1^T \mathbf{V}_2 dS, \tag{44}$$

the governing equations (31) projected onto a POD mode $\boldsymbol{\phi}_m$ and with the application of the adiabatic wall boundary condition on $\partial\Omega_W$:

$$(\boldsymbol{\phi}_m, \mathbf{A}_0\mathbf{V}_{,t}) - \left(\boldsymbol{\phi}_{m,i}, \tilde{\mathbf{A}}_i\mathbf{V}\right) - \left(\boldsymbol{\phi}_m, \tilde{\mathbf{A}}_{i,i}\mathbf{V}\right) + (\boldsymbol{\phi}_{m,i}, \tilde{\mathbf{K}}_{ij}\mathbf{V}_{,j}) \underbrace{-\langle \boldsymbol{\phi}_m, [\tilde{\mathbf{A}}_i n_i \mathbf{V}]^{np} \rangle_{\partial\Omega_W}}_{=I_m^{np}} + \underbrace{\langle \boldsymbol{\phi}_m, [\tilde{\mathbf{K}}_{ij}^\nu n_i \mathbf{V}_{,j}]^{ns} \rangle_{\partial\Omega_W}}_{=I_m^{ns}} = 0. \tag{45}$$

The no-slip (28) and no-penetration (29) boundary conditions are implemented weakly by substituting these boundary conditions into the boundary integral terms in (45), namely $I_m^{ns}$ and $I_m^{np}$, respectively. Substituting the modal expansion (42) into (45), the following ODE system is obtained:

$$\begin{aligned}\textstyle\sum_{n=1}^M (\boldsymbol{\phi}_m, [\mathbf{A}_0]_M \boldsymbol{\phi}_n)\dot{a}_n \quad &= \left(\boldsymbol{\phi}_{m,i}, [\tilde{\mathbf{A}}_i]_M \mathbf{V}_M\right) + \left(\boldsymbol{\phi}_m, [\tilde{\mathbf{A}}_{i,i}]_N \mathbf{V}_M\right) - (\boldsymbol{\phi}_{m,i}, [\tilde{\mathbf{K}}_{ij}]_M \mathbf{V}_{M,j}) + \langle \boldsymbol{\phi}_m, [\tilde{\mathbf{A}}_i n_i \mathbf{V}]_M^{np} \rangle_{\partial\Omega_W} \\ &\quad - \langle \boldsymbol{\phi}_m, [\tilde{\mathbf{K}}_{ij}^\nu n_i \mathbf{V}_{,j}]_M^{ns} \rangle_{\partial\Omega_W}.\end{aligned} \tag{46}$$

Here, $[\mathbf{A}_0]_M \equiv \mathbf{A}_0(\mathbf{V}_M) = \mathbf{A}_0\left(\sum_{n=1}^M a_n(t)\boldsymbol{\phi}_n\right)$ and similarly for the other matrices with "$M$" subscripts in (46).

The non-linearity in the full Navier-Stokes equations (22) is in the advection term, or Euler fluxes $\mathbf{A}_i$. Note, however, that the diffusive terms in the entropy variable analog of (22), namely (31), are also non-linear, due to the fact that the symmetrizing matrix (Jacobian) $\mathbf{A}_0 \equiv \mathbf{U}_{,\mathbf{V}}$ is a function of $\mathbf{V}$. Hence, *all* the symmetrized matrices, namely $\tilde{\mathbf{A}}_i$ and $\tilde{\mathbf{K}}_{ij}$ are non-linear in $\mathbf{V}$. Note also that, since $\mathbf{A}_0 \equiv \mathbf{A}_0(\mathbf{V})$, although the basis functions satisfy $(\boldsymbol{\phi}_j, \boldsymbol{\phi}_i) = \delta_{ij}$ for any $i, j = 1,...M$, they are not $\mathbf{A}_0$-orthogonal, that is,

$$(\boldsymbol{\phi}_i, \mathbf{A}_0\boldsymbol{\phi}_j) \neq \delta_{ij}. \tag{47}$$

A consequence of (47) is a mass matrix will appear in the semi-discrete ROM to be advanced forward in time (see e.g., (48)).

As discussed earlier, the ROM (46) is not efficient due to the presence of multiple strong non-linearities. Efficiency can be recovered by applying the best-points interpolation procedure described earlier in Section 3. With interpolation, the ROM system (46) takes on the form:

$$\mathbf{M}\dot{\mathbf{a}}_M = \mathbf{G}^{\mathbf{f}_i}\mathbf{f}_i(\mathbf{D}^{\mathbf{f}_i}\mathbf{a}_M) + \mathbf{G}^4\mathbf{f}_4(\mathbf{D}^{\mathbf{f}_4}\mathbf{a}_M) - \mathbf{G}^{\mathbf{f}_{i+4}}\mathbf{f}_{i+4}(\mathbf{D}^{\mathbf{f}_{i+4}}\mathbf{a}_M) - \mathbf{G}^{\mathbf{f}_8}\mathbf{f}_8(\mathbf{D}^{\mathbf{f}_8}\mathbf{a}_M) - \mathbf{G}^{\mathbf{f}_9}\mathbf{f}_9(\mathbf{D}^{\mathbf{f}_9}\mathbf{a}_M), \tag{48}$$

where the matrices $\mathbf{G}^{\mathbf{f}_i}$ and $\mathbf{D}^{\mathbf{f}_i}$ are defined by analogy to (20)[4]. (48) can be advanced in time using a standard explicit time-integration scheme, or an implicit time-integration scheme, with the application of Newton's method at each time step. It is emphasized again that the upshot of formulating the ROM *with* interpolation is all the inner-products are contained in the $\mathbf{G}^{\mathbf{f}_j}$ matrices in (48), which can be pre-computed prior to time integration of and/or application of Newton's method to the ROM ODE system (48). Similarly, the interpolated mass matrix $\mathbf{M}$ can also be pre-computed. The time-integration of the ROM ODE system (48) requires the inversion of this matrix, but since the number of modes $M$ will in general be quite small, the relative cost of this inversion is minuscule.

# 6 Preliminary Numerical Study: Burgers' Equation

Prior to building the reduced order model formulated and shown to be entropy-stable for the compressible Navier-Stokes equations (Section 5), it is useful to perform a preliminary numerical study to gauge the viability of the POD basis, an empirical basis, for non-linear fluid problems possessing features like weak shocks and rarefactions, both of which are supported by solutions of the equations (22). A much simpler canonical prototype problem whose solutions may exhibit these same features is the viscous Burgers' equation. Consider the following initial boundary value problem (IBVP) for Burgers' equation:

$$\begin{aligned} &u_t + \left(\tfrac{u^2}{2}\right)_x = \mu u_{xx}, \qquad -1 < x < 3, \quad 0 < t < T, \\ &u(-1,t) = u(3,t) = 0, \qquad\qquad\qquad\quad 0 < t < T, \end{aligned} \tag{49}$$

with initial condition

$$u(x,0) = \begin{cases} 0, & x < 0, \\ 1, & 0 \le x < 1, \\ 0, & x \ge 1, \end{cases} \tag{50}$$

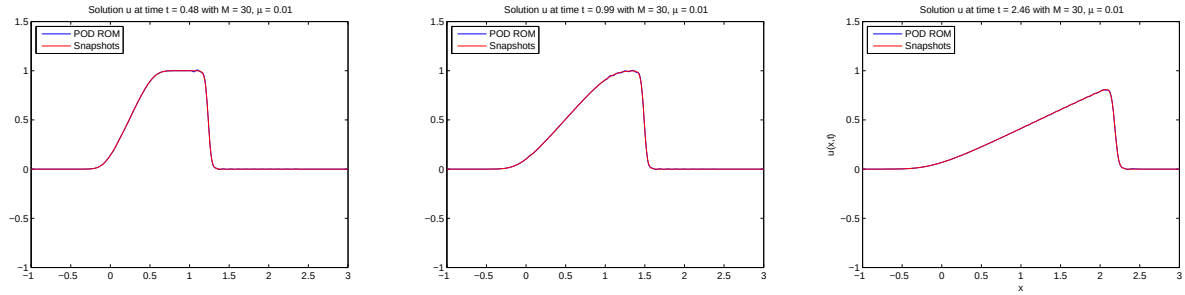
Discontinuous initial data (50) are specified such that both a rarefaction and a shock form in the $\mu \to 0$ limit.

A POD/Galerkin ROM for (49) with initial condition (50) was constructed from a high-fidelity solution (discretized with a third order ENO-LLF method in space and fourth order Runge-Kutta method in time), with $\Delta x = 0.008$. A total of $K = 101$ snapshots of this solution were taken, at increments $\Delta t_{snap} = 0.03$, up to time $T = 3$. Both the POD basis and Galerkin projection for (49) were defined in the $L^2(\Omega)$ inner product[5].

Figs. 1–2 show the computed ROM solution using a POD basis with $M = 30$ without and with the "best points" interpolation respectively. The spacing of the interpolation points computed via the BPIM method of [14, 15] and outlined in Section 3 is reasonable given the character of the exact solution to this problem (Fig. 2 (a)). Both ROMs are able to capture the essential features of the solution, namely the weak shock and rarefaction. Minor oscillations are apparent in the vicinity of the weak shock. This suggests that the

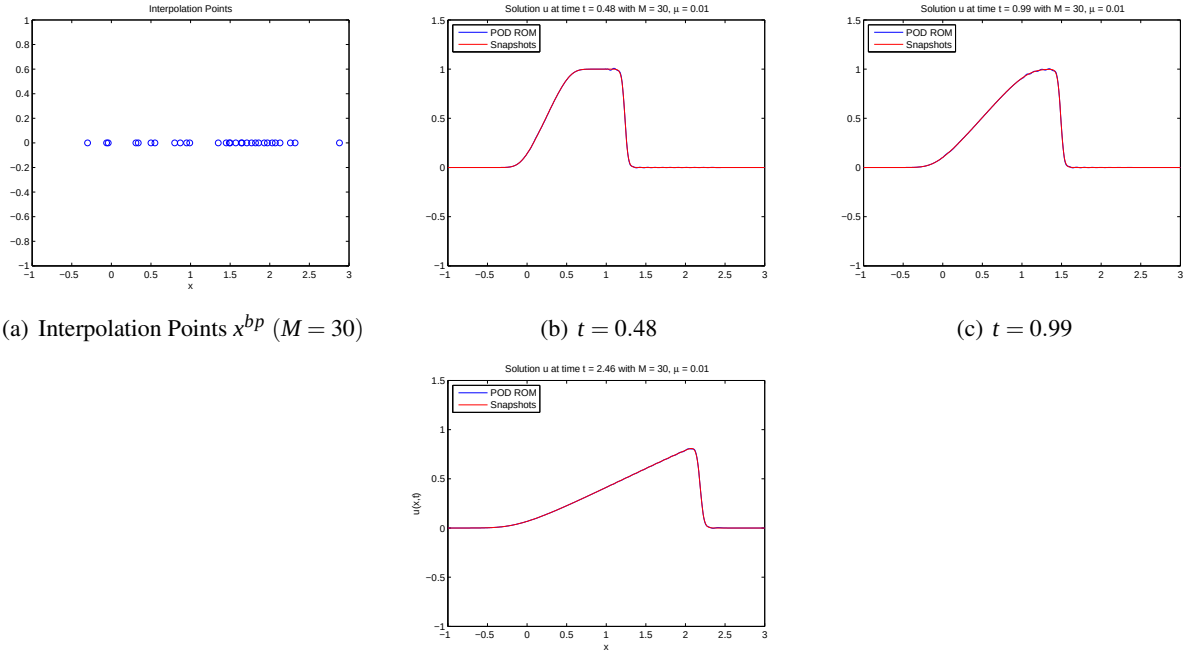
[4] Explicit expressions for the matrices that appear in (48) will be given in the final conference paper manuscript.

[5] An energy stability result can be shown for the Galerkin projection of the one-dimensional (1D) viscous Burgers' equation on $\Omega = (x_0, x_1) \subset \mathbb{R}$ in the $L^2$ inner product (44), under certain conditions on the boundary conditions, including those in (49).




(a) $t = 0.48$ (b) $t = 0.99$ (c) $t = 2.46$

Figure 1: POD ROM solution to Burgers' IBVP (49) with $M = 30$ (no interpolation)




(a) Interpolation Points $x^{bp}$ $(M = 30)$ (b) $t = 0.48$ (c) $t = 0.99$

(d) $t = 2.46$

Figure 2: POD ROM solution to Burgers' IBVP (49) with $M = 30$ (with "best points" interpolation)

addition of some artificial viscosity may be required [4, 16] when $\mu$ is small to capture accurately the shock. We hope to solicit insight regarding the viability of POD bases for non-linear conservation law problems, as well as stabilization and shock-capturing approaches in reduced order modeling, at the conference. The final paper manuscript will include results for other conservation laws whose solutions possess weak shocks.

Table 1: Fluid variables

| Variable | Physical Meaning | Expression |
|---|---|---|
| $\rho$ | fluid density | |
| $u_i$ | fluid velocity in the $i^{th}$ direction | |
| $\delta_{ij}$ | Kronecker delta | $\delta_{ij} = 1$ if $i = j$, $\delta_{ij} = 0$ otherwise |
| $e$ | total energy density | $e = \imath + \frac{1}{2}u^2$ |
| $\imath$ | internal energy density | $\imath = c_v\theta$ |
| $\theta$ | absolute temperature | |
| $c_v$ | specific heat at constant volume | |
| $c_p$ | specific heat at constant pressure | |
| $\gamma$ | ratio of specific heats | $\gamma = c_p/c_v$ |
| $p$ | fluid pressure | $p = (\gamma-1)\rho\imath$ |
| $\tau_{ij}$ | viscous stress | $\tau_{ij} = \lambda u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i})$ |
| $\lambda$, $\mu$ | viscosity coefficients | |
| $q_i$ | heat flux | $q_i = -\kappa\theta_{,i}$ |
| $\kappa$ | conductivity | |
| $\eta$ | thermodynamic entropy density per unit mass | |
| $s$ | nondimensional entropy | $s \equiv \eta/c_v = \ln(p\rho^{-\gamma}) + \text{const}$ [Gibbs' equation] |
| $t$ | time | |
| $\mathbf{x}$ | position vector in Cartesian coordinates | $\mathbf{x}^T = (x_1, x_2, x_3)$ |

# Appendix

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